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Hydrogen Storage: Thermochemical Studies of N-Alkylcarbazoles and Their Derivatives as a Potential Liquid Organic Hydrogen Carriers

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Abstract

© 2015 American Chemical Society. Although N-ethylcarbazole is considered as a most promising potential liquid organic hydrogen carriers (LOHC) substance, a major drawback for stationary and particularly mobile applications is its high melting point of 343 K. Study of other possible N-alkylcarbazole-derivatives having lower melting points but keeping a high storage density is of practical importance. This contribution presents thermochemical properties (enthalpy of formation, enthalpy of vaporization, enthalpy of sublimation, and fusion enthalpy) for N-alkylcarbazoles (with alkyl = isopropyl, n-propyl, and n-butyl) derived from experiments in order to investigate the applicability of the carbazole derivatives as potential LOHCs. Additionally, high-level quantum chemical calculations were applied to determine molar enthalpies of formation of the gaseous carbazole derivatives and thus validated the experimental findings. Using a combination of the quantum-chemical calculations with vaporization enthalpy data measured in this work, the standard molar liquid phase enthalpies of formation were derived for alkylcarbazole derivatives. Results of this study were applied for thermodynamic analysis of the liquid-phase reversible hydrogenation/dehydrogenation processes with N-alkylcarbazoles.

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